=> file registry
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

TOTAL

ENTRY 0.84

SESSION 1.05

FILE 'REGISTRY' ENTERED AT 12:14:05 ON 15 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 JUN 2004 HIGHEST RN 693217-50-4 DICTIONARY FILE UPDATES: 14 JUN 2004 HIGHEST RN 693217-50-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\10072641.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1

STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sam

SAMPLE SEARCH INITIATED 12:14:33 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 19 TO ITERATE

100.0% PROCESSED

19 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

119 TO 641

PROJECTED ITERATIONS: PROJECTED ANSWERS:

0 TO

Ĺ2

0 SEA SSS SAM L1

=> s l1 full sss

FULL SEARCH INITIATED 12:15:00 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 349 TO ITERATE

100.0% PROCESSED

349 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

3 SEA SSS FUL L1

=> d scan str

3 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN Absolute stereochemistry.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

3 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN Absolute stereochemistry.

L3 3 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

Absolute stereochemistry.

ALL ANSWERS HAVE BEEN SCANNED

=> d his

L1

(FILE 'HOME' ENTERED AT 12:07:59 ON 15 JUN 2004)

FILE 'REGISTRY' ENTERED AT 12:08:05 ON 15 JUN 2004 E 5-AMINO-2'-DEOXYURIDINE-5'-TRIPHOSPHATE/CN

FILE 'REGISTRY' ENTERED AT 12:14:05 ON 15 JUN 2004

STRUCTURE UPLOADED

L2 0 S L1 SAM

L3 3 S L1 FULL SSS

=> file caplus
COST IN U.S. DOLLARS

OST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 156.26 157.31

FILE 'CAPLUS' ENTERED AT 12:15:57 ON 15 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 15 Jun 2004 VOL 140 ISS 25 FILE LAST UPDATED: 14 Jun 2004 (20040614/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 9 L3

=> s 14 and composition

616552 COMPOSITION

273258 COMPOSITIONS

884631 COMPOSITION

(COMPOSITION OR COMPOSITIONS)

1282412 COMPN

513247 COMPNS

1569642 COMPN

(COMPN OR COMPNS).

2003604 COMPOSITION

(COMPOSITION OR COMPN)

0 L4 AND COMPOSITION

.=> d fbib abs hitstr total 14

L4 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:777381 CAPLUS

DN 139:273245

TI Uridihe analogs and techniques for making and using

IN Verdine, Gregory L.; Storek, Michael

PA USA

L5

SO U.S. Pat. Appl. Publ., 16 pp.

CODEN: USXXCO

DT Patent

LA English FAN.CNT 1

PATENT NO. KIND DATE

APPLICATION NO. DATE

US 2002-72641 20020207 US 2002-72641 20020207

PI US 2003186930 A1 20031002

Uridine analogs and techniques for making and using uridine analogs are disclosed in this invention. These uridine analogs include nucleoside phosphates having a 5-aminouracil group. These nucleotides can be incorporated into a nucleic acid as an unnatural base, as a substitute for uridine or thymine. The nucleic acid can then be treated with an oxidizing agent and an alkaline solution, which causes cleavage of the nucleic acid at the position of the unnatural base. The nucleoside phosphate analogs can be used in many ways, including measuring chemical interactions between nucleic acids and other compds, or sequencing nucleic acids. Addnl. compds. can also be derivitized onto the amino group, allowing other functionalities to be added to the nucleoside phosphate; or to the nucleic acid incorporating the nucleoside phosphate.

IT 113980-89-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

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RN
     113980-89-5 CAPLUS
     Uridine 5'-(tetrahydrogen triphosphate), 5-amino-2'-deoxy- (9CI)
Absolute stereochemistry.
  ΗŅ
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      NH_2
     ANSWER 2 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
L4
AN
     2003:696404
                  CAPLUS
DN
     139:208773
     Genotyping methods for detection of single nucleotide polymorphisms using
ΤI
     base-modified oligonucleotides in nucleic acid amplification
     Wolfe, Jia Liu; Kawate, Tomohiko; Allerson, Charles R.; Stanton, Vincent
IN
PΑ
     U.S. Pat. Appl. Publ., 30 pp., Cont.-in-part of U.S. (6,566,059
SO
     CODEN: USXXCO
     Patent
DT
LA
     English
FAN.CNT 6
     PATENT NO.
                       KIND
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              CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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(uridine analogs and techniques for making and using)

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US 1998-102724PP 19981001

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US 2000-709596 A320001109
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FAN
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                                                US 2000-709596 A320001109
AB
     The present invention relates to a method for genotyping a diploid
     organism to detect single nucleotide polymorphisms (SNPs) using modified nucleotides or nucleotide residues substituted with fluorescent groups.
     The present invention comprises replacing a natural nucleotide with a
     base-modified nucleotide in a polynucleotide, and subsequently cleaving
     the polynucleotide with a chemical base. In this work, the bases consisted
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of secondary amines with high b.ps., and included 3-pyrrolidinol, 2-pyrrolidinemethanol, 3-pyrrolidinemethanol, 4-hydroxypiperidine and 4-piperidineethanol. In the examples, this method is used in genotyping allele variations in the genes encoding the transferrin receptor and cytochrome P 4502D6. Particularly useful aspects of this method are ease of assay design, low cost of reagents and suitability of the cleavage

products for detection by a variety of methods.

10/035753

IT 113980-89-5

RL: ARG (Analytical reagent use); DGN (Diagnostic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(genotyping methods for detection of single nucleotide polymorphisms using base-modified oligonucleotides in nucleic acid amplification)

RN 11/3980-89-5 CAPLUS

CN Uridine 5'-(tetrahydrogen triphosphate), 5-amino-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:760649 CAPLUS

DN 1/38/12330

TI 5-Amino-2'-deoxyuridine, a Novel Thymidine Analogue for High-Resolution Footprinting of Protein-DNA Complexes

AU Storek, Michael J.; Suciu, Alexandru; Verdine, Gregory L.

CS Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138., USA

SO Organic Letters (2002), 4(22), 3867-3869 10/31/2002 CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

OS CASREAGT 138:12330

AB 5-Amino-2'-deoxyuridine 5'-triphosphate, an analog of deoxythymidine triphosphate, was synthesized and found to be a substrate of Taq DNA polymerase. The DNA-borne analog underwent selective chemical reaction with permanganate. The use of 5-amino-dU as an interference probe was validated using the Ada protein/ada promoter complex. The performance of 5-amino-dU in interference footprints is similar to that of the previously described analog 5-hydroxy-dU, but the former is incorporated more readily into DNA during enzymic polymerization

IT 113980-89-5P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(base pair with adenine; 5-amino-2'-deoxy\ridine 5'-triphosphate interferes with formation of Ada protein-DNA complex for high-resolution footprinting)

RN 113980-89-5 CAPLUS

CN Uridine 5'-(tetrahydrogen triphosphate), 5-amino-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN L4

AN 1997:591303 CAPLUS

DN 127, 278403

Preparation of oligonucleotides containing non-natural base analogs TΙ

ΑU Eritja, Ramon; Adam, Viviane; Avino, Anna; Diaz, Antonio R.; Fabrega, Carme; Ferrer, Elisenda; Grotli, Morten; Guimil Garcia, Ramon; Hofmann, Mechtild; Marquez, Victor E.; Wiersma, Marten European Molecular Biol. Lab., Heidelberg, D-69117, Germany

CS

SO Nucleosides & Nucleotides (1997), 16(5 & 6), 697-702 CODEN: NUNUD5; ISSN: 0732-8311

PB Dekker

Journal DT

English LA

The preparation of oligonucleotides containing 5-amino-2'-deoxyuridine, AΒ 5-N-acetamido-2'-deoxyuridine, 5-aza-2'-deoxycytidine and N2-substituted guanosine derivs. is described. In each case selection of the appropriate protective group, synthesis and deprotection conditions is discussed.

IT194412-17-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of oligodeoxyribonucleotides containing non-natural base

analogs)

194412-17-4 CAPLUS RN

Uridine, 2^{1} -deoxyadenylyl- $(3^{1}\rightarrow 5^{1})$ -5-amino-2'-deoxy- (9CI) CN INDEX NAME)

Absolute stereochemistry.

RE.CNT THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD 14 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN AN 1997:520073 CAPLUS

DN 127/:205808

TI Synthesis of oligodeoxynucleotides containing 5-aminouracil and its N/acetyl derivative

AU Ferrer, Elisenda; Neubauer, Gitte; Mann, Matthias; Eritja, Ramon CS European Molecular Biology Laboratory, Heidelberg, D-69117, Germany SO Journal of the Chemical Society, Perkin Transactions 1: Organic and

Bio-Organic Chemistry (1997), (14), 2051-2057 CODEN: JCPRB4; ISSN: 0300-922X

Royal Society of Chemistry

DT Journal

PΒ

LA English

The preparation of oligonucleotides containing 5-amino-2'-deoxyuridine is described. Three different protective groups for the amino function of 5-aminouracil including trifluoroacetyl, dimethylformamidine and 2-(4-nitrophenyl)ethoxycarbonyl are analyzed in order to reduce the acetylation of this base observed during the assembly of oligonucleotides containing this base analog. The side-reaction is avoided by using the base-labile 2-(4-nitrophenyl)ethoxy as protecting group and 2-(4-nitrophenyl)ethyl chloroformate during the capping step.

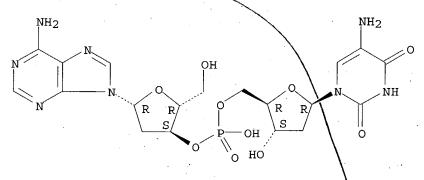
IT 194412-17-4P

RL:\SPN (Synthetic preparation); PREP (Preparation)
(preparation of aminouracil-containing oligodeoxyribonucleotides)

RN 194412-17-4 CAPLUS

CN Uridine, 2'-deoxyadenylyl-(3'→5')-5-amino-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry



RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1988:164220 CAPLUS

DN 108:164220

TI Nonradioactive labeling of synthetic oligonucleotide probes with terminal deoxynucleotidyl transferase

AU Kumar, Abhay; Tchen, Paul; Roullet, Francoise; Cohen, Jean

CS Stn. Rech. Virol. Immunol., INRA, Thiverval Grignon, F-78850, Fr.

SO Analytical Biochemistry (1988), 169(2), 376-82, CODEN: ANBCA2; ISSN: 0003-2697

DT Journal

LA English

AB Synthetic oligonucleotides were tailed at the 3' end using terminal deoxynucleotidyl transferase. Nucleotide triphosphates with free primary amines at the end of side chains were compared for their tailing efficiency and/or detection sensitivity, using biotin-11-dUTP as a reference Free primary amines were tagged with activated biotin or fluorescein isothiocyanate. The probes were then detected with either

streptavidin-alkaline phosphatase complex or anti-fluorescein antibodies and alkaline phosphatase-conjugated secondary antibodies. Tailing conditions were optimized and the probes were tested for detection of Escherichia coli ST1a enverotoxin DNA and rotavirus RNA.

IT 113980-89-5

RL: ANST (Analytical study)

(oligonucleotide labeling by terminal deoxynucleotidyl transferase with)

RN 113980-89-5 CAPLUS

CN Uridine 5'-(tetrahydrogen triphosphate), 5-amino-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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ANSWER 7 OF 9
                     CAPLUS COPYRIGHT 2004 ACS on STN
L4
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AN
                  CAPLUS
     107:115932
DN
     5-Azidodeoxyuridine compounds
TI
IN
     Haley, Boyd E.; Evans, Robert K.
PΑ
     University of Wyoming, USA
SO
     PCT Int. Appl., 25 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                       KIND
                             DATE
                                             APPLICATION NO.
                                                               DATE
ΡI
     WO 8606253
                        A1
                             19861106
                                             WO 1986-US854
                                                               19860422
         BW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE
                                             US 1985-726145
                                                               19850423
     US 4672111
                        Α
                             19870609
                                             US 1985-726145
                                                               19850423
     EP 218701
                       Α1
                             1987042/2
                                             EP 1986-902752
                                                               19860422
     EP 218701
                        B1
                             19930804
         R: CH, DE, FR, GB, LI, SE
                                             US 1985-726145
                                                               19850423
     CA 1266643
                        A1
                             19900313
                                             CA 1986-507355
                                                               19860423
                                             US 1985-726145
                                                               19850423
os
     CASREACT 107:115932
GΙ
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$$M^{+} \begin{bmatrix} 0 \\ 0 \\ - \\ 0 \\ - \\ 0 \end{bmatrix} = 0$$

$$CH_{2}$$

$$R_{1}$$

$$R$$

The title nucleosides and nucleotides [I; R = H, OH; R1 = (PO42-)m, H, OH; n = 1-5; m = 1-3; M+ = mono- or divalent cation], useful for preparation of photoactive DNA in photoaffinity labeling of DNA, were prepared Thus, treatment of 2'-deoxyuridine 5'-monophosphate with NOBF4 and Zn reduction of the resulting 5-nitro-2'-deoxyuridine 5'-monophosphate gave 5-amino-2'-deoxyuridine-5' monophosphate which was diazotized by NaNO2 in 1N HCl and treated with NaN3 to give 5-azido-2'-deoxyuridine 5'-monophosphate. This was activated with (PhO)2P(O)Cl in DMF and treated with tetrabutylammonium pyrophosphate to give 5-azido-2'-deoxyuridine 5'-triphosphate which was a good substrate of DNA polymerase (no data) to produce photoactive DNA.

IT 4603-58-1P

RL: RCT (Réactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant ϕ r reagent)

(preparation and diazotization of)

Ι

RN 4603-58-1 CAPLUS

CN 5'-Uridylic acid, 5-amino-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1987:46270 CAPLUS

DN 106:462 \(\)0

on 113

TI Synthesis and biological properties of 5-azido-2'-deoxyuridine 5'-triphosphate, a photoactive nucleotide suitable for making light-sensitive DNA

AU Evans, Robert K.; Haley, Boxd E.

CS Dep. Microbiol./Biochem., Univ. Wyoming, Laramie, WY, 82071, USA

SO Biochemistry (1987), 26(1), 269-76 CODEN: BICHAW; ISSN: 0006-2960 DT Journal

LA English

AB A photoactive nucleotide analog of dUTP, 5-azido-2'-deoxyuridine 5'-triphosphate (5-N3dUTP), was synthesized from dUMP in 5 steps. The key reaction in the synthesis of 5-N3dUTP is the nitration of dUMP in 98% yield in 5 min at 25° by an excess of nitrosonium tetrafluoroborate in anhydrous DMF. Reduction of the resulting 5-nitro compound with Zn and 20

mM

HCl gave \$\frac{4}{3}\$-aminodeoxyuridine monophosphate (5-NH2dUMP). Diazotization of 5-NH2dUMP with HNO2 followed by the addition of NaN3 to the acidic diazonium salt solµtion gave a photoactive nucleotide derivative in 80-90% yield. The monophosphate product was identified as 5-N3dUMP by proton NMR, UV, IR, and chr ϕ matog. anal. as well as by the mode of synthesis and by its photosensitivity. After formation of 5-N3dUTP through a chemical coupling of pyrophosphate to 5-N3dUMP, the triphosphate form of the nucleotide was found to support DNA synthesis by Escherichia coli DNA polymerase I at a rate inf qistinguishable from that supported by dTTP. When UMP was used as the starting compound, 5-aminouridine triphosphate (5-N3UTP) was prepared in an analogous fashion with similar yields and produced a photoactive nucleotide which is a substrate for E. coli RNA polymerase. To prepare $[\gamma-32P]$ 5-N3dUTP for use as an active-site-directed photoaffinity labeling reagent, a simple method of preparing γ -32P-labeled pyrimidine nucleotides was developed. [γ -32P]5-N3dUTP is an effective photoaffinity labeling reagent for DNA polymerase I; it bound to the active site with a 2-fold higher affinity than dTTP. The photoactivity of 5-N3dUMP is stable to extremes of pH, and $[\gamma-32P]5-N3dUTP$ is an effective photolabeling reagent even in the presence of 10 mM dithiothreitol. 5-Azidouracil-containing nucleotides have potential applications as active-site-directed photoaffinity labeling reagents and as tools for generating photoactive DNA and RNA to study nucleic acid-binding proteins.

IT 4603-58-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and diazotization of)

RN 4603-58-1 CAPLUS

CN 5'-Uridylic acid, 5-amino-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

on IO

L4 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1986:622031 CAPLUS

DN 105:222031

TI 5-Azido-2'-deoxyuridine 5'\triphosphate: a photoaffinity-labeling reagent and tool for the enzymic synthesis of photoactive DNA

AU Evans, R. K.; Johnson, J. D \backslash ; Haley, B. E.

CS Lucille Parker Markey Cancer\Cent., Univ. Kentucky, Lexington, KY, 40536,

USA

SO Proceedings of the National Academy of Sciences of the United States of America (1986), 83(15), 5382-6 CODEN: PNASA6; ISSN: 0027-8424

DT Journal LA English

AB The photoactive deoxyuridine nucleotide 5-azido-2'-deoxyuridine 5'-triphosphate (5-N3dUTP) was prepared and used it to synthesize pight-sensitive DNA by enzymic incorporation. In the absence of UV light, 6-N3dUTP is a substrate for Escherichia coli DNA polymerase I. In in Witro DNA synthesis reactions using bacteriophage M13 single-stranded DNA as the template and 5-N3dUTP in place of dTTP, a photoactive complementary strand was not synthesized when the 5-N3dUTP was substituted for dCTP or when it was exposed to UV light prior to the addition of DNA polymerase I. Using a synthetic lac operator template of 26 bases and a 15-base primer, we generated a\photoactive 26-base-pair lac operator by enzymically incorporating 5-N3dUMP with DNA polymerase I. Crosslinking of this photoactive DNA fragment to lac repressor was totally dependent on the presence of UV light and was reduced 78% by 150 μM iso-Pr β -D-thiogalactoside. Under the same conditions no crosslinking to lac repressor was observed using a nonphotoactive 26-base-pair lac operator. Photoactivable deoxyuridine analogs have potential application as reagents to crosslink DNA binding proteins to 5-azidouracil-containing DNA and as active-site-directed photoaffinity labeling reagents.

IT 4603-58-1

RL: ANST (Analytical study)

(azotization of)

RN 4603-58-1 CAPLUS

CN 5'-Uridylic acia, 5-amino-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.